International Journal of Mass Spectrometry 352 (2013) iii–v

Contents lists available at ScienceDirect

International Journal of Mass Spectrometry

journal homepage: www.elsevier.com/locate/ijms

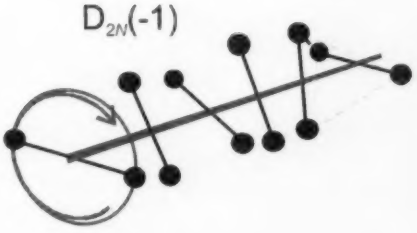
Contents

1–8

Excitation levels in ultra-dense hydrogen p(−1) and d(−1) clusters: Structure of spin-based Rydberg Matter

Leif Holmlid

● The novel theory for ultra-dense materials predicts that several excitation levels of spin quantum number s exist. ● A theoretical description of superconductors by J.E. Hirsch is the starting point. ● The agreement with the normal experimental D–D distance is excellent at 2.23 pm for $s = 2$. ● The predicted inter-atomic distance is only 0.56 pm in the lowest excitation level $s = 1$. ● Theory is verified by experimentally detecting states with spin values $s = 1$ and $s = 3$.

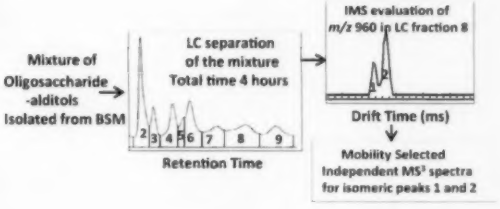


9–18

Evaluation of ion mobility-mass spectrometry for determining the isomeric heterogeneity of oligosaccharide-alditols derived from bovine submaxillary mucin

Hongli Li, Brad Bendiak, Kimberly Kaplan, Eric Davis, William F. Siems, Herbert H. Hill Jr.

● Ion mobility-mass spectrometry (IMMS) has the capability to rapidly evaluate the isomeric heterogeneity of oligosaccharide mixtures on millisecond timescale. ● Even after a single HPLC column, isomeric structures that were present in fractions could frequently be resolved as independent peaks using IMMS. ● Ion mobility coupled to tandem stages of mass spectrometry enabled different sets of product ions to be assigned to different isomeric precursors within a given *m/z* pool.

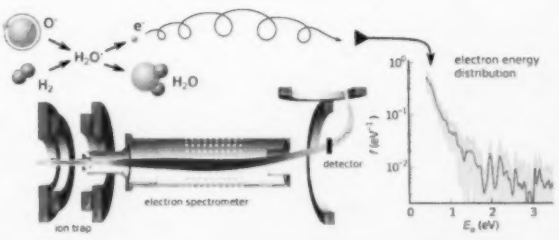


19–28

Determining the energy distribution of electrons produced in associative detachment: The electron spectrometer with multipole trap

P. Jusko, Š. Roučka, R. Plašil, J. Glosík

● Instrument for measuring the energy of electrons produced in ion trap. ● Calibration with electrons from photodetachment. ● Energy distribution of electrons from associative detachment.



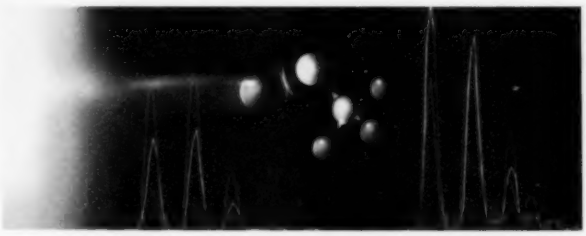
Elsevier B.V.
http://dx.doi.org/10.1016/S1387-3806(13)00344-8

29–36

Probing Ni^+ metastable state production in sputtering glow discharges with the use of diagnostic reactions

William S. Taylor, Kendall G. Fancher, Li Chen Chen, Benjamin K. Ward, Casey A. Cameron

● Ion mobility spectrometry indicates Ni^+ ($3d^9$) and Ni^+ ($3d^84s^1$) in d.c. discharges. ● Charge-transfer bracketing indicates Ni^+ states as high as ^2P. ● Evidence for additional excited states below ^2P is observed. ● Excited Ni^+ state distributions are independent of the discharge gas.

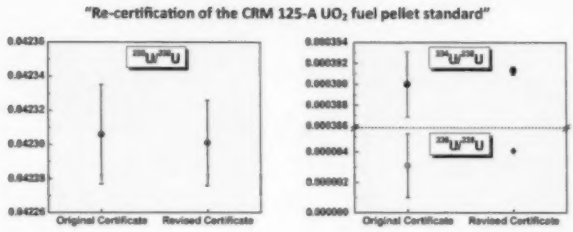


37–43

Re-certification of the CRM 125-A UO_2 fuel pellet standard for uranium isotopic composition

M. Kraiem, R.M. Essex, K.J. Mathew, G.J. Orlowicz, M.D. Soriano

● CRM 125-A is a 5.4 g UO_2 pellet assay and isotopic standard (4% enriched in ^{235}U). ● The CRM 125-A UO_2 pellet is being developed as a CRM for U–Th age determinations. ● The U isotopic composition is determined by TIMS using 3 independent methods. ● Re-certification of CRM 125-A has resulted in significantly smaller uncertainties for the U minor isotope-amount ratios. ● The revised values for CRM 125-A are provided in a new certificate of analysis.

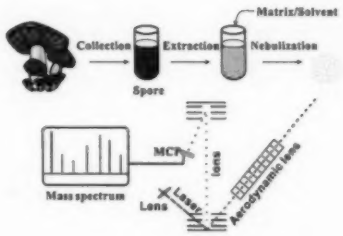


44–50

Differentiation of basidiospores by MALDI-TOF lipid profiling

Yueyan Li, Miao Liang, Xi Shu, Changgeng Liu, Jinian Shu

● Lipid profiles of six basidiospores were obtained with MALDI-TOF MS. ● Sample preparation strategies of the MALDI analyses were optimized. ● Phospholipids, diacylglycerols, and triacylglycerols were observed.

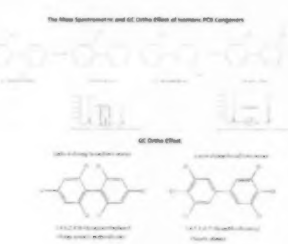


51–64

The mass spectrometric ortho effect studied for all 209 PCB congeners

L.I. Osemwengie, G.W. Sovocool

● PCB mass spectra can provide structural information beyond mw and no. of Cls. ● 2,2′- and 2,2′, 6-substitution show largest effects in mass spectra. ● Chlorine loss fragment (ortho effect) studied for all 209 congeners. ● Combined with complementary chromatographic ortho effect. ● Permits recognition of incorrect structural assignments.

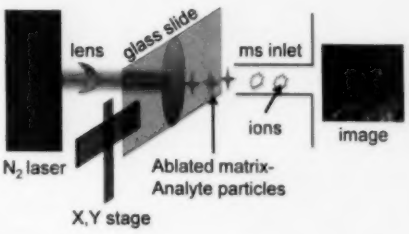


65–69

High mass resolution tissue imaging at atmospheric pressure using laserspray ionization mass spectrometry

Andrew F. Harron, Khoa Hoang, Charles N. McEwen

● Tissue imaging of lipids, peptides, small proteins, and drugs are demonstrated using laserspray ionization at 100,000 mass resolution. ● Images of low abundance ions show that most originate from the tissue and are not matrix background ions. ● Simultaneous imaging of a peptide, protein, and lipids are achieved with delipified tissue. ● Three lipids are imaged within a mass window of 0.07 Da.

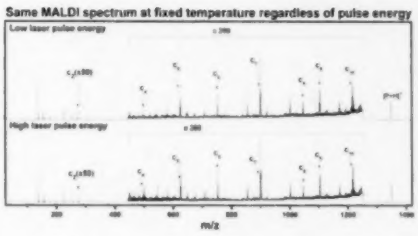


70–76

Thermal determination of the abundances of c and z type fragment ions generated by in-source decay of peptide ions in matrix-assisted laser desorption ionization

Kyung Man Park, Yong Jin Bae, Jeong Hee Moon, Myung Soo Kim

● MALDI spectrum of a peptide is thermally determined whether ISD of its molecular ion occurs via b–y or c–z mechanism. ● If hydrogen atoms participate in the c–z mechanism, they are generated by X–H bond cleavage in the ground electronic state. ● A linear calibration curve is obtained for a peptide whose molecular ion dissociates mainly via c–z channels.

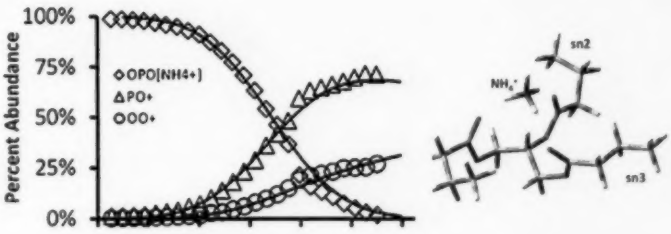


77–86

Energy and entropy at play in competitive dissociations: The case of uneven positional dissociation of ionized triacylglycerides

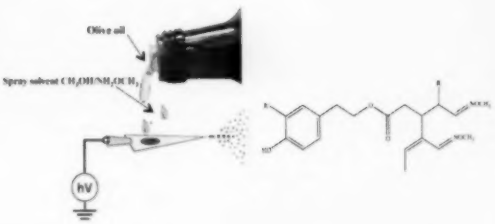
Justin B. Renaud, Sean Overton, Paul M. Mayer

● We have explored the competing dissociation of TAG-NH_4^+ adduct ions. ● Competition between sn-1,3 and sn-2 position bond cleavage due to energy and entropy effects. ● Sn1,3 fatty acid cleavage is energetically favourable. ● Sn2 fatty acid cleavage is entropically favoured.



87–91

Evaluation of dialdehydic anti-inflammatory active principles in extra-virgin olive oil by reactive paper spray mass spectrometry

Fabio Mazzotti, Leonardo Di Donna, Domenico Taverna, Monica Nardi, Donatella Aiello, Anna Napoli, Giovanni Sindona

● Direct analysis by paper spray, without sample preparation. ● In situ derivatization and identification of dialdehydic species. ● Evaluation of anti-inflammatory active principles.